Scaling and Universality in the Anisotropic Kondo Model and the Dissipative Two-State System

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Scaling and universality in the Ohmic two-state system is investigated by exploiting the equivalence of this model to the anisotropic Kondo model. For the Ohmic two-state system, we find universal scaling functions for the specific heat $C_\alpha(T)$, static susceptibility $\chi_\alpha(T)$, and spin relaxation function $S_\alpha(\omega)$, depending on the reduced temperature T/Δ_r (frequency ω/Δ_r), with Δ_r the renormalized tunneling frequency, and uniquely specified by the dissipation strength α ($0 < \alpha < 1$). The scaling functions can be used to extract α and Δ_r in experimental realizations. [S0031-9007(97)05207-1]

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The low energy effective model for a large number of physical systems corresponds to a two-state system coupled to an environment [1,2]. Examples include two-level atoms coupled to the electromagnetic field in quantum optics, electron-transfer reactions in biological systems, and the tunneling of defects in metallic glasses [3]. The simplest model for describing such systems is the spin-boson Hamiltonian [1],

$$H_{SB} = -\frac{1}{2}\Delta\hat{\sigma}_x + \frac{1}{2}\epsilon\hat{\sigma}_z + \sum_i \omega_i\left(a_i^\dagger a_i + \frac{1}{2}\right) + \frac{1}{2}q_0\hat{\sigma}_z\sum_i \frac{C_i}{\sqrt{2m_i\omega_i}}(a_i + a_i^\dagger). \quad (1)$$

Here the Pauli matrices $\hat{\sigma}_i, i = x, y, z$ describe the two-level system, Δ is the bare tunneling matrix element between the states $\sigma_z = \uparrow$ and $\sigma_z = \downarrow$ and ϵ is a bias. The environment is represented by an infinite set of harmonic oscillators (labeled by the index i) with masses m_i and frequency spectrum ω_i linearly coupled to the coordinate $Q = \frac{1}{2}q_0\sigma_z$ with coupling constants C_i. In this paper we restrict ourselves to Ohmic dissipation, for which the environment spectral function $J(\omega) = \frac{\pi}{2}\sum_i(\frac{C_i^2}{m_i\omega_i})\delta(\omega - \omega_i)$ takes the form $J(\omega) = 2\pi\alpha\omega$, for $\omega \ll \omega_c$, where ω_c is a high energy cutoff and α is a dimensionless coupling constant characterizing the strength of the dissipation. The two dimensionless couplings of the model are Δ/ω_c and α: in this paper we consider the region of parameter space, $\Delta/\omega_c \ll \alpha < 1$, which includes the interesting case of a nonadiabatic bath.

The Ohmic spin-boson model has been intensively investigated over the last ten years [1,2]. The main interest has been in understanding how the environment influences the dynamics of the two-level system and in particular how dissipation destroys quantum coherence [1,2,4–7]. Insight has been gained by exploiting the equivalence of the Ohmic two-state system to several other models, including the inverse square Ising model [4], the anisotropic Kondo model (AKM) [5], and the resonant level model [8–10]. The qualitative picture that has emerged can be summarized as follows. There is a renormalized tunneling frequency Δ_r, which depends on α and Δ, and which decreases monotonically with increasing α for fixed Δ. For $\alpha = 0$, $\Delta_r = \Delta$ (decoupled system plus bath) and for $\alpha > 0$ the renormalization of this scale increases dramatically as the dissipation strength is increased to 1: $\Delta_r/\omega_c \sim (\Delta/\omega_c)^{1/1-\alpha}$. Between $\alpha = 0$ and $\alpha = 1$, there is a range of different behavior from coherent oscillations at zero dissipation to damped oscillations at intermediate dissipation strengths and eventually to incoherent relaxation at strong dissipation [1,2]. At $\alpha > \alpha_c(\Delta) \approx 1$ there is a "localization" transition at $T = 0$ corresponding to a vanishing renormalized tunneling frequency $\Delta_r = 0$ [11]. Here we address one aspect which has not been dealt with in a unified way in the literature, namely, the meaning of universality and scaling in these models, in particular, for physical properties, such as thermodynamic and dynamical quantities. We apply Wilson's numerical renormalization group (NRG) method to the AKM to calculate the specific heat, static susceptibility, and dynamical susceptibility. The equivalence of the two models then allows us to discuss scaling and universality in the dissipative two-state system.

The AKM [12] is given by

$$H = \sum_{k,\sigma}\epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \frac{J_\perp}{2}\sum_{kk'}(c_{k\uparrow}^\dagger c_{k'\downarrow}S^- + c_{k\downarrow}^\dagger c_{k'\uparrow}S^+) + \frac{J_\parallel}{2}\sum_{kk'}(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow})S^z + g\mu_B h S_z, \quad (2)$$

where the first term represents noninteracting conduction electrons and the second and third terms represent an exchange interaction between a localized spin $1/2$ and the conduction electrons with strength $J_\perp, J_\parallel$. A local magnetic field, h, coupling only to the impurity spin in the Kondo model [the last term in Eq. (2)] corresponds to a finite bias, ϵ, in the spin-boson model. The correspondence between H and H_{SB}, established via bosonization [9], implies $\epsilon = g\mu_B h$, $\frac{\Delta}{\omega_c} = \rho_0 J_\perp$, and $\alpha = (1 + \frac{2\delta}{\pi})^2$, where $\tan\delta = -\frac{\pi\rho_0 J_\parallel}{4}$. δ is the phase shift for scattering of electrons from a potential $J_\parallel/4$ and $\rho_0 = 1/2D_0$ is the conduction electron density of states per spin at the Fermi level for a flat band of width $2D_0$ [1,5,9]. We

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choose $\omega_c = 2D_0$ so that $\Delta = J_\perp$ and measure all energies relative to $D_0 = 1$. Since we are interested in describing the Ohmic two-state system for $\Delta/\omega_c \ll \alpha < 1$, this requires in the AKM that $\rho_0 J_\perp \ll 1 - \rho_0 J_\parallel$ for $\rho_0 J_\parallel \ll 1$ ($\alpha \to 1^-$ case) and $\rho_0 J_\perp \ll 1/(\rho_0 J_\parallel)^2$ for $\rho_0 J_\parallel \gg 1$ ($\alpha \to 0$ case). The AKM for $\rho_0 J_\perp > \rho_0 J_\parallel$ will be dealt with elsewhere, so in effect we consider only $\rho_0 J_\perp \ll \min(\rho_0 J_\parallel, \alpha)$.

We solve the AKM using Wilson's NRG method [13]. In this procedure, a separation of energy scales is made by introducing a logarithmic mesh of k points $k_n = \Lambda^{-n}$, $\Lambda > 1$, and transforming the $c_{k\sigma}$ to a basis of Wannier states $f_{n\sigma}$ [13] at the impurity, with $f_{0\sigma} = \sum_k c_{k\sigma}$, such that $H_c = \sum_{k\mu} \epsilon_{k\mu} c^\dagger_{k\mu} c_{k\mu}$ is tridiagonal in k space, i.e., $H_c \to \sum_\mu \sum_{n=0}^\infty \Lambda^{-n/2} (f^\dagger_{n+1\mu} f_{n\mu} + \text{H.c.})$. The Hamiltonian (2) in the new basis is now diagonalized by defining a sequence of finite size Hamiltonians H_N containing the first N Wannier states together with the impurity. One diagonalizes the rescaled Hamiltonians $\bar{H}_N = \Lambda^{\frac{N-1}{2}} H_N$ which satisfy the recursion relation $\bar{H}_{N+1} = \Lambda^{1/2} \bar{H}_N + \sum_\mu (f^\dagger_{N+1\mu} f_{N\mu} + \text{H.c.})$. This gives the excitations and eigenstates at a corresponding set of energy scales ω_N defined by $\omega_N = \Lambda^{-\frac{N-1}{2}}$ and allows the calculation of dynamic quantities at frequencies $\omega \sim \omega_N$ and thermodynamic quantities at temperatures $k_B T_N \sim \omega_N$. For example, the Fourier transform of $\chi(t,T) = -i\theta(t)\langle[S_z(t), S_z(0)]\rangle$ is given by $\chi(\omega,T) = \chi'(\omega,T) + i\chi''(\omega,T) = \frac{1}{Z_N} \sum_{m,n} |M^N_{m,n}|^2 \frac{e^{-\beta\epsilon_m} - e^{-\beta\epsilon_n}}{\omega + i0 - (\epsilon_m - \epsilon_n)}$, where ϵ_m, ϵ_n are excitations of H_N, $Z_N(T)$ the partition function of H_N, and $M^N_{m,n} = \langle m|S_z|n\rangle_N$.

Specifically, for the AKM we calculate (a) the $T = 0$ relaxation function $S(\omega) = -\frac{1}{\pi} \frac{\chi''(\omega + i\delta)}{\omega}$, (b) the impurity specific heat $C(T) = -T\partial^2 F_{\text{imp}}/\partial T^2$, where the impurity free energy is given by $F_{\text{imp}}(T) = -k_B T \ln Z/Z_0$ and Z_0 is the conduction electron partition function, and (c) the local static susceptibility $\chi'(\omega = 0, T)$ corresponding to setting the g factor of the conduction electrons to zero. Under the equivalence, the operator $\sigma_z/2$ of the spin-boson model translates to S_z in the AKM, so $S(\omega)$ gives the relaxation function for the spin-boson problem. We extract the local static susceptibility, $\chi_{\text{sb}}(T) = -(1/\beta)(\partial^2 \ln Z_{\text{sb}}/\partial \epsilon^2)_{\epsilon=0}$, of the Ohmic spin-boson model from $\chi'(\omega = 0, T)$ at finite T. Finally, the decoupling of spin and charge degrees of freedom in the AKM allows identification of F_{imp} as the free energy of the spin-boson model (with bath contribution subtracted) and of $C(T)$ as the corresponding specific heat.

The energy level flow diagram for some low lying rescaled energy states is shown in Fig. 1. We see that spin-rotational invariance, which is broken for $J_\perp \neq J_\parallel$ at high energies, is restored below the low energy scale of the model, the Kondo temperature $T_K(J_\perp, J_\parallel)$ [15], leading to the well known isotropic strong coupling fixed point at low energies (e.g., the lowest single particle states in Fig. 1, $\eta_1 = 0.6555, \eta_2 = 1.976$ agree with the $\Lambda = 2$ results of [13]). A detailed analysis [16] gives $T_K \sim (\Delta/\omega_c)^{1/(1-\alpha)}$ with Δ, α related to $J_\perp, J_\parallel$ as above and $J_\perp \ll J_\parallel$ and a prefactor also depending on α, i.e., T_K has the same dependence on α as the low energy scale Δ_r. The flow to the isotropic strong coupling fixed point holds for any initial anisotropy, corresponding to $0 < \alpha < 1$, with the flow being *universal* for each α [16]: the energy levels for fixed α and different $\Delta/\omega_c \ll \alpha$ may be shifted onto each other by a translation in N [17], except for a small "transient" region $N \sim 0$–10 corresponding to high energies $\omega \gg \Delta_r$ near the cutoff ω_c. We see that the energy level flow is uniquely specified by two parameters, Δ_r (equivalently T_K) which sets the crossover scale in Fig. 1, and the dissipation strength α (or equivalently the dimensionless initial coupling constant $\rho_0 J_\parallel$). The universal flow of energy levels is the origin of the scaling, for fixed α and arbitrary $\Delta/\omega_c \ll \alpha$, in the thermodynamic quantities we discuss below [18].

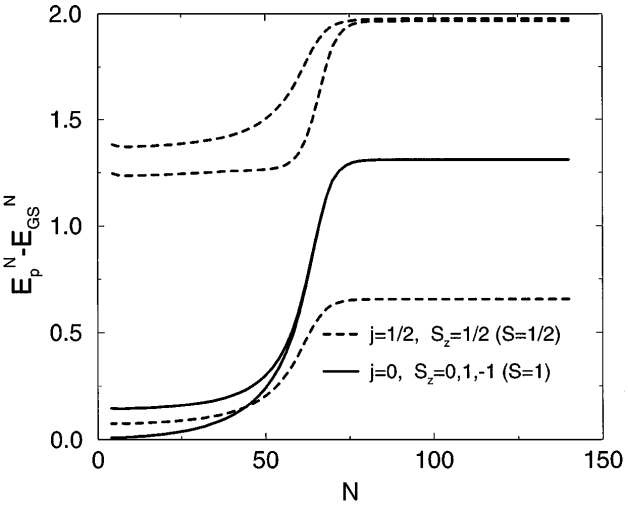

FIG. 1. The lowest rescaled energy levels for even N iterations for $J_\parallel = 0.443$ and $J_\perp = 0.010$ [5] corresponding to $\Delta = 0.01$ and $\alpha = 0.8$ in the spin-boson model. The energy levels are labeled by the conserved quantum numbers, total pseudospin j [14], and total z component of spin S_z. There is a crossover to the strong coupling fixed point at iteration N_c corresponding to $\Lambda^{-(N_c-1)/2} \approx \Delta_r = T_K$. Spin rotational invariance is restored at low energies (e.g., the $j = 0$ states with $S_z = 0$ and $S_z = \pm 1$ become degenerate), so the states at the strong coupling fixed point can be labeled by total spin S as indicated.

The inset in Fig. 2 shows that the specific heat curves for $\alpha = 0.2$ and several values of Δ all scale onto a universal curve corresponding to $\alpha = 0.2$. For different α one obtains distinct universal curves, $C_\alpha(T)$ (Fig. 2). Scaling is valid for all temperatures in the range $k_B T \ll D_0$, not only at low temperatures $k_B T \ll \Delta_r = T_K$. In Fig. 2, and throughout this paper, we scale the temperature by $\alpha/\gamma = 3\Delta_r/\pi^2 k_B^2$. This follows from an exact result for the Wilson ratio [8,19] discussed below together with our *definition* $\chi_{\text{sb}}(0) = 1/2\Delta_r$. The specific heat is linear in temperature for $k_B T \ll \Delta_r$ and $0 < \alpha < 1$, with a linear coefficient γ in good agreement with values

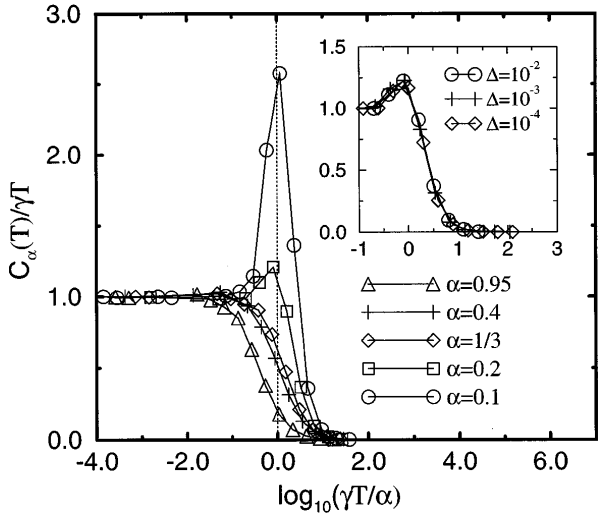

FIG. 2. Universal specific heat curves, $\frac{C_\alpha(T)}{\gamma T}$, for the Ohmic two-state system for $0 < \alpha < 1$. $\gamma = \lim_{T\to 0} C(T)/T \sim \alpha/\Delta_r$ is extracted from the fixed point analysis [16]. The symbols represent the temperatures at which the numerical second derivative of $F_{\rm imp}$ has been calculated. The inset is for $\alpha = 0.2$.

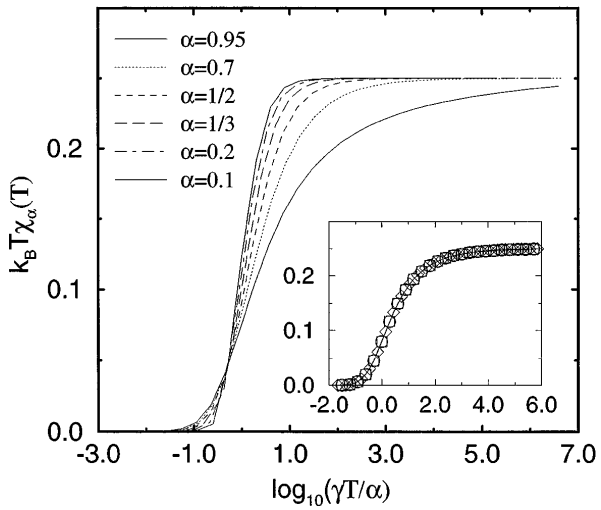

FIG. 3. Universal curves for the static susceptibility of the Ohmic two-state system, $k_B T\chi_\alpha(T)$, for $0 < \alpha < 1$, with $\gamma \sim \alpha/\Delta_r$ as in Fig. 2. The inset is for $\alpha = 0.8$ and $\Delta = 0.005$ ($\circ$), $\Delta = 0.05$ ($\Box$), and $\Delta = 0.01$ ($\diamond$).

extracted from an analysis of the strong coupling fixed point [16]. This is also expected from the Fermi liquid ground state of the model. We note that the T^3 coefficient of the specific heat changes sign close to $\alpha = 1/3$, corresponding to the appearance, for weak dissipation, of damped oscillations at frequency Δ_r [5,6]. The peak in $C(T)/T$ can be taken as a signature of a two-level system weakly coupled to bosonic excitations—it is absent for strong Ohmic dissipation. The strong dependence of $C(T)/T$ on α for weak dissipation is also seen in other quantities, such as in the spin response [5].

The universal curves for the static susceptibility, $\chi_\alpha(T)$, parametrized by the dimensionless dissipation strength, α, are shown in Fig. 3. The inset shows that curves with the same $\alpha = 0.8$ and different Δ scale onto the same curve for $k_B T \ll D_0$. The thermodynamic calculation for χ_α becomes inaccurate at low temperatures, $k_B T \ll \Delta_r$ (discussed in detail in [5,16]), and we have to resort to an analysis about the strong coupling fixed point. This yields a finite susceptibility at $T = 0$ which is accurate to within 1% for $0 < \alpha < 1$ (see Table I below and [16]). At high temperatures, $\Delta_r \ll k_B T \ll D_0$, there is a dramatic difference in the approach of $k_B T\chi_\alpha(T)$ to its free spin value of $1/4$ between the cases of weak and strong dissipation. In the former, the free spin value is reached very rapidly on increasing the temperature above Δ_r. The logarithmic terms characterizing the slow approach of $k_B T\chi_\alpha(T)$ to the free spin value in the Kondo case are small for weak dissipation and only set in when $\alpha \to 1^-$. In this limit and for $\Delta/\omega_c \ll 1$, the scaling functions for the Kondo problem are recovered for the specific heat and static susceptibility [16].

A universal Wilson ratio for the AKM [8] has been proven also for the Ohmic and non-Ohmic spin-boson models [19]. For the Ohmic case, the Wilson ratio for the spin-boson model, $R_{\rm sb} = \lim_{T\to 0} \frac{4}{3} \frac{\pi^2 k_B^2}{(g\mu_B)^2} \frac{T\chi_{\rm sb}}{C} = 2/\alpha$ [19]. This is related to the Wilson ratio, $R_{\rm akm} = \lim_{T\to 0} \frac{4}{3} \frac{\pi^2 k_B^2}{(g\mu_B)^2} \frac{T\chi_{\rm akm}}{C} = 2$, for the AKM [8] by $R_{\rm sb} = R_{\rm akm}/\alpha$ since $\chi_{\rm sb} = \chi_{\rm akm}/\alpha$ [8] and $\chi_{\rm akm}$ is the susceptibility of the AKM (with a g factor of 2 for the conduction electrons). Table I shows that $R_{\rm akm} = 2$ ($R_{\rm sb} = 2/\alpha$) is recovered for $\Delta/\omega_c \ll \alpha$ and $0 < \alpha < 1$.

Dynamical quantities also show the universality discussed above for thermodynamic quantities. The $T = 0$ relaxation functions, $S(\omega)$, for dissipation strength $0 < \alpha < 1$ have been given in [5]. A detailed analysis shows that these are universal functions of ω/Δ_r parametrized by α: $S = S_\alpha(\omega/\Delta_r)$. The case of $\alpha = 1/3$, corresponding to the crossover between damped oscillations and incoherent relaxation [5,6,20], is shown in Fig. 4. Scaling in $S_\alpha(\omega)$ extends to all frequencies $\omega \ll D_0$ and is not restricted to $\omega \lesssim \Delta_r$. At high frequencies, $\omega \gg \Delta_r$, we obtain $S_\alpha(\omega) \sim \omega^{-(4-2\alpha)}$; thus $\chi''(\omega) \sim \omega^{-(3-2\alpha)}$ and $C_s(t) \equiv \langle[\sigma_z(t), \sigma_z(0)]_-\rangle \sim 1 - ct^{2(1-\alpha)}$ for $D_0^{-1} \ll t \ll \Delta_r^{-1}$ with the α dependent exponents being accurate to within 0.1% for $0 < \alpha < 1$. These results agree with short-time approximations [1] and perturbative methods [9] in this limit. More importantly, they indicate that scaling, in the sense discussed in this paper, can be

TABLE I. γ, $\chi_{\rm akm}$, and $R_{\rm akm}$, extracted from the fixed point analysis.

α	$\Delta = J_\perp$	$\chi_{\rm akm}$	γ	$R_{\rm akm}$
10^{-3}	10^{-6}	489.2	3214.6	2.003
10^{-3}	10^{-4}	4.78	30.76	2.04
$1/3$	0.01	275.1	1806.1	2.005
$1/3$	0.1	8.61	56.4	2.01
0.7	0.01	1.90×10^6	1.25×10^7	2.002
0.9	0.1	1.81×10^6	1.19×10^7	2.003

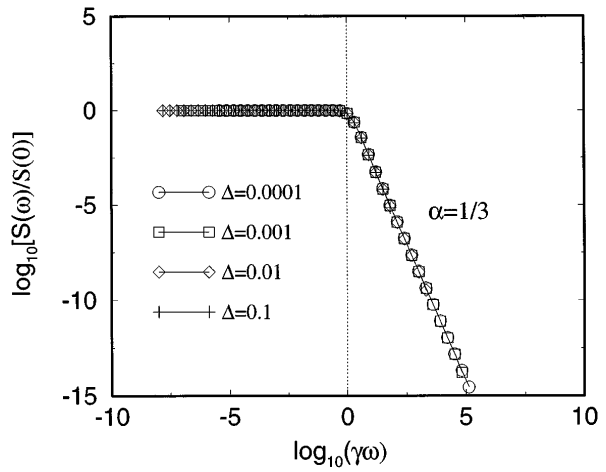

FIG. 4. Universal curve for the relaxation function $S_\alpha(\omega)$.

expected only for fixed α. At low frequencies, $\omega \ll \Delta_r$, the Fermi liquid behavior of $\chi''(\omega, T = 0) \sim \alpha\omega$ gives $C_s(t) \sim -\alpha/t^2$, with an α independent *exponent* for $t \gg 1/\Delta_r$ [4,5,19].

Deviations from scaling, starting at high temperatures and frequencies, set in on increasing Δ/ω_c for our finite bandwidth model. The scaling discussed here is valid for $0 < \alpha < 1$ ($0 < J_\parallel < \infty$) as long as Δ/ω_c remains the smallest bare energy scale.

The scaling and universality discussed above can be useful in interpreting experiments on dissipative two-state systems. The dissipation strength α can be determined by fitting the data for some quantity, such as $S(\omega)$, to the appropriate universal scaling function $S_\alpha(\omega)$. The low energy scale, Δ_r, can be extracted from the low energy/temperature behavior [e.g., from $S_\alpha(\omega)$ by using the generalized Shiba relation [19] $S_\alpha(0) = 2\alpha[\chi_{\rm sb}(T = 0)]^2$ and $\chi_{\rm sb}(T = 0) = 1/2\Delta_r$]. In practice, this may be difficult for strong dissipation $\alpha \geq 1/3$ since the scaling functions for different α will differ appreciably only for $k_B T, \omega > \Delta_r$. In this case an alternative is to extract α and Δ_r from $\gamma = \pi^2 k_B^2 \alpha/3\Delta_r$ and $\chi_{\rm sb} = 1/2\Delta_r$. α and Δ_r can be more easily deduced for weakly dissipative systems $\alpha < 1/3$, for which the scaling functions depend sensitively on α, even for $k_B T, \omega \ll \Delta_r$.

To summarize, we have used the equivalence of the Ohmic spin-boson model to the AKM in order to study universality and scaling in these models. For anisotropies in the AKM, $0 < J_\perp \ll J_\parallel < +\infty$, corresponding to dissipation strengths $0 < \alpha < 1$ and bare tunneling frequencies $\Delta/\omega_c \ll \alpha$ in the Ohmic spin-boson model, the thermodynamic (dynamic) properties of these models are characterized by universal scaling functions of T/Δ_r (ω/Δ_r) which are *distinct* functions for different α and are independent of Δ—the latter entering only through Δ_r. As in the Kondo problem, the scaling functions are universal with deviations from scaling at high frequencies and temperatures arising from finite Δ/ω_c. The dissipation strength in the Ohmic two-state system, just as the anisotropy in the AKM, determines the essential physics, in particular, the renormalization of the low energy scale $\Delta_r/\omega_c \sim (\Delta/\omega_c)^{1/(1-\alpha)}$ and the form of the scaling functions. The perspective gained above may also be useful in understanding the highly anisotropic multichannel Kondo models which arise in the context of single electron devices, and two-level systems in solids interacting with electrons [21].

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[18] This is consistent with the Bethe ansatz for the AKM [15] where the scaling trajectories are labeled by a parameter which we can relate to α for $0 < \alpha < 1$ and $\Delta/\omega_c \ll \alpha$ [16]. Renormalizations of α, entering the scaling functions, are typically a fraction of a percent [being $O((\Delta/\omega_c)^2)$] and unimportant in the regime of interest for the Ohmic two-state system studied in this paper.
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